Laboratory Name: Idaho National Laboratory
B&R Code: KC 0202010

FWP and possible subtask under FWP: 100390
Structural and Electrostatic Effects in Self Assembled Nanostructure and Interface Growth.
FWP Number: 3E106 (100390)
Program Scope: This work was originally part of a Field Work Proposal (FWP) that contained two Tasks; a research Task and the quarter time detailee Task. At the request of the Office of Basic Energy Sciences, the detailee Task is being written up as a new FWP. The basic research Task, outlined in the following, is focused on obtaining a better understanding of nanoparticles and of interfaces between, for example, compound semiconductors and other materials. Such an understanding of the interfaces between nanostructures and their substrates, and between heteroepitaxied materials, is of considerable interest both in terms of increasing our fundamental knowledge and of facilitating our ability to synthesize these important systems. In FY2006, a new component was added to this work to explore the dynamic behavior of nanoparticles ranging in size from tens to thousands of atoms. The phenomena under investigation include sublimation, sintering and related behavior dependent upon the nanoparticle binding energy. The primary approach used in this work is the comparison of experimental data with model caculations, and the use of model calculations to explore new systems for which detailed experimental data is not available. Theoretical studies will use first-principles, density functional theory calculations and other formalisms.
Major Program Achievements (over duration of support):
Publications for 2006:

1. "Nonequilibrium Phases in Epitaxial Mn/GaAs Interfacial Reactions", H. H. Farrell, J. L. Hilton, B. D. Schultz and C. J. Palmstrøm, submitted to Journal of Vacuum Science and Technology, B24, 2018.

2. “Diatomic substitutionals in superconducting Nb(1-x)B2”, H. H. Farrell, R. A. LaViolette and T. M. Lillo, Physica C – Superconductivity and its applications, 449, 1, 2006.

(Funded in part through residual CS&P funds.)

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This research Task is subdivided into four components; a.) Semiconductor interfaces and nanostructure, (including vacancies), b.) Oxide/semiconductor interfaces, c.) Dynamics at metastable interfaces and d) Dynamic behavior of nanoparticles. The primary effort in FY2006 was focused on developing the last, and newest, componenet. The binding energy of a wide variety of nanoparticles was determined. For "good" metals, this was shown to be inversely dependent on the particle size. For "poor" metals and covalently bonded materials, the dependence is more complex. In the former case, a simple expression for vapor pressure and related phenomena was developed. In FY2007 and FY2008, it is anticipated that work on all four components will proceed. The effort on the semiconductor interfaces will continue in collaboration with Prof. C. J. Palmstrom, U. of Minn., The oxide/semiconductor component will be resumed in collaboration with Prof. D. Schlom, Penn. State U., when he returns from sabbatical later in 2007. The studies of metastable interfaces will continue in collaboration with Dr. C. D. Van Siclen, INL. Work on the dynamics of nanoparticles will continue in collaboration with Dr.s D. M. Ginosar, L. M. Petkovic and S. Rashkeev of INL.
Program impact:
The work performed under this task is designed to increase our understanding of the forces that shape the detailed atomic nature of surfaces and interfaces under both equilibrium and non-equilibrium conditions.
Interactions:
Idaho National Laboratory (C. D. Van Siclen, D. M. Ginosar, L. M. Petkovic, S. Rashkeev);
University of Minnesota at Minneapolis (C. J. Palmstrom);
Pennsylvania State University (Darrell Schlom).
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Committee; Physics and Chemistry of Semiconductor Surfaces Annual Meetings.
Personnel Commitments for FY2005 to Nearest +/- 10%:
Helen H. Farrell, 50 %
Authorized Budget (BA) for FY03, FY04, FY05:
FY04 BA $272K FY05 BA $265K FY06 BA $ 200 K